COMPUTER SIMULATIONS OF SODIUM LAURETH SULPHATE WORMLIKE MICELLES

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Wormlike micelles (WLM) can be formed by surfactant systems at moderate concentrations and are found in personal care products. WLMs are long, flexible structures that share many features with traditional polymeric systems, but an important difference is that they can break and reform. This similarity to polymers forms the basis of a theoretical description developed by Cates and co-workers[1] that relates the microscale structure to the macroscopic properties. One key parameter is the scission free energy, E_{sci}, that is, the change in free energy upon breaking a cylindrical micelle into two hemispherical caps (see Figure 1). This can be directly related to the mean micelle length and the viscosity.

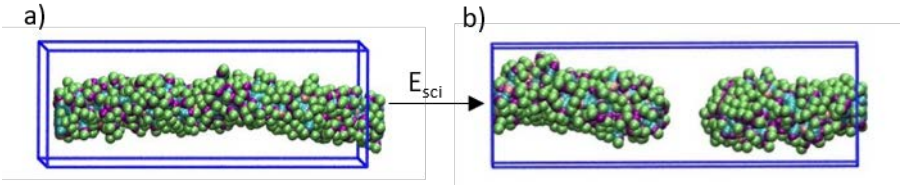

Figure 1 The scission free energy (E_{sci}) is the change in energy from breaking a wormlike micelle (a) into two wormlike micelles with hemispherical caps (b).

Here we use Dissipative Particle Dynamics simulations to calculate E_{sci} for WLMs of sodium laureth sulphate (SLES), a key ingredient in many personal care products via the protocol developed by Wang *et al* [2]. Briefly, we simulate an infinitely long micelle and calculate E_{sci} using umbrella sampling. From these simulations we are investigating how the salt concentration and surfactant attributes (head group size, alkyl tail length) affect E_{sci}. We find that E_{sci} increases with increasing salt content indicating longer micelles are present, in agreement with previous literature results[2]. However, upon increasing the alkyl chain length from C12 to C16, a 4-fold increase in E_{sci} and a qualitatively different potential of mean force is observed.

[1] M. E. Cates and S. J. Candau, J. Phys. Condens. Matter, 2, 6869 (1999)

[2] H. Wang, X. Tang, D. M. Eike, R. G. Larson and P. H. Koening, Langmuir, 34, 1564-1573 (2018)

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